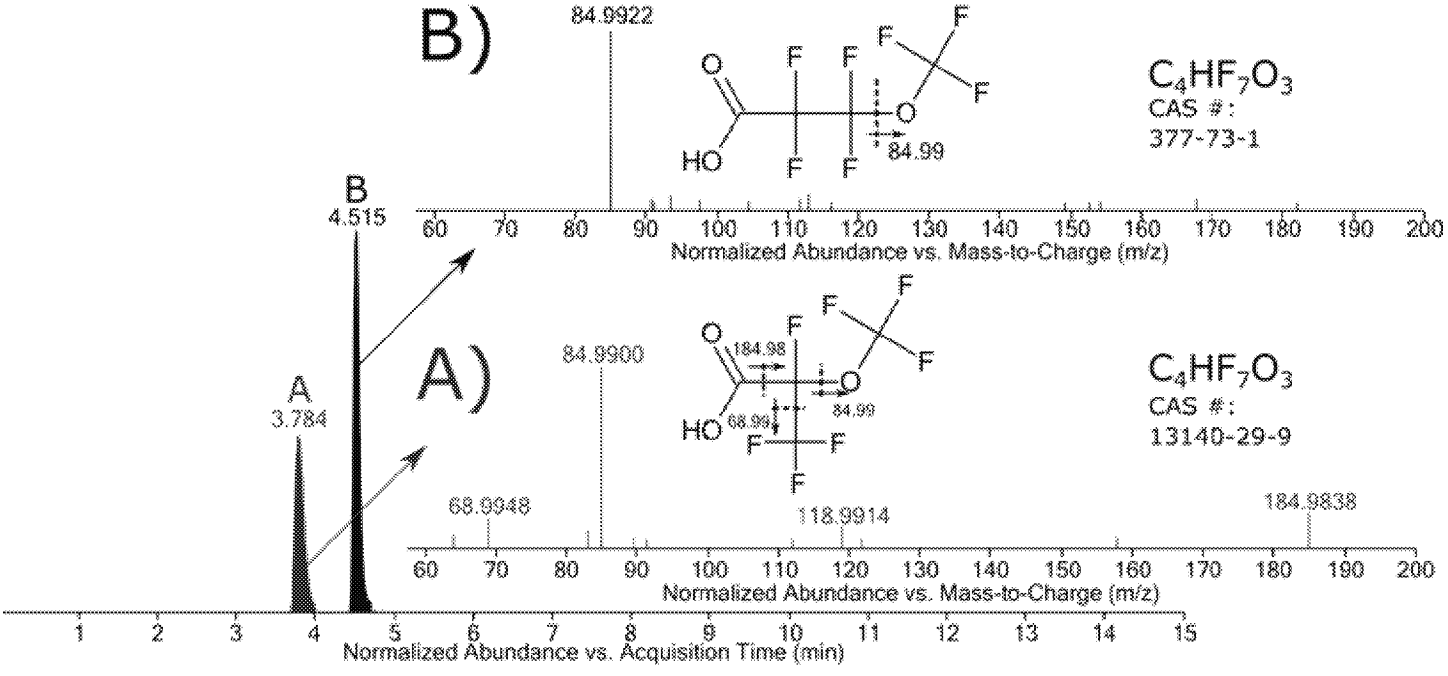
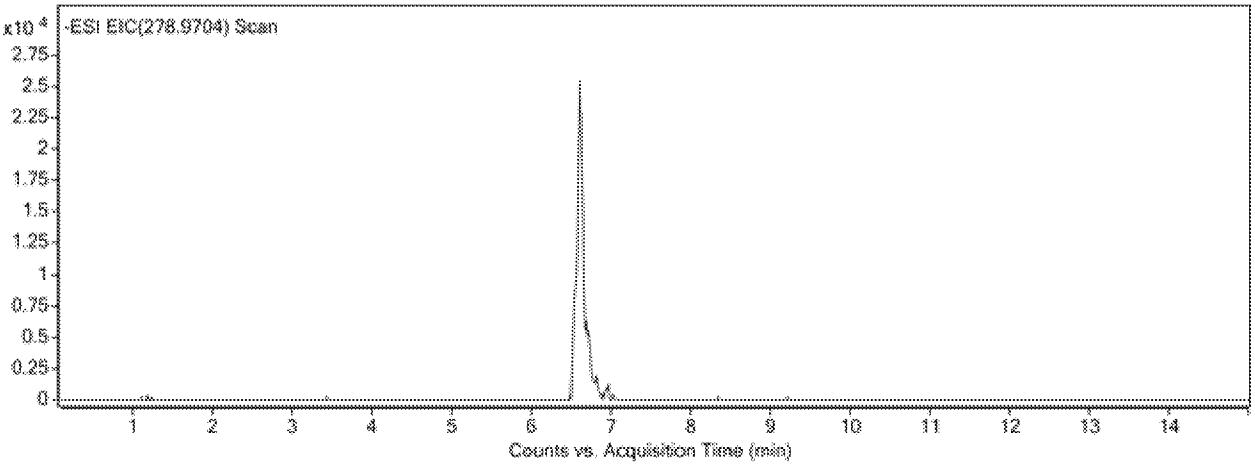
Message

From: McCord, James [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=MCCORD, JAMES]
Sent: 5/25/2018 12:13:33 PM
To: Detlef R. U. Knappe [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=user17c3f77b]; Strynar, Mark [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a9910d5b38e471497bd875fd329a20a-Strynar, Mark]
CC: Hopkins, Zachary [zrhopkin@ncsu.edu]; Nadine Kotlarz [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=userc79d3fb6]; Chuhui Zhang [czhang24@ncsu.edu]
Subject: RE: Package Delivery

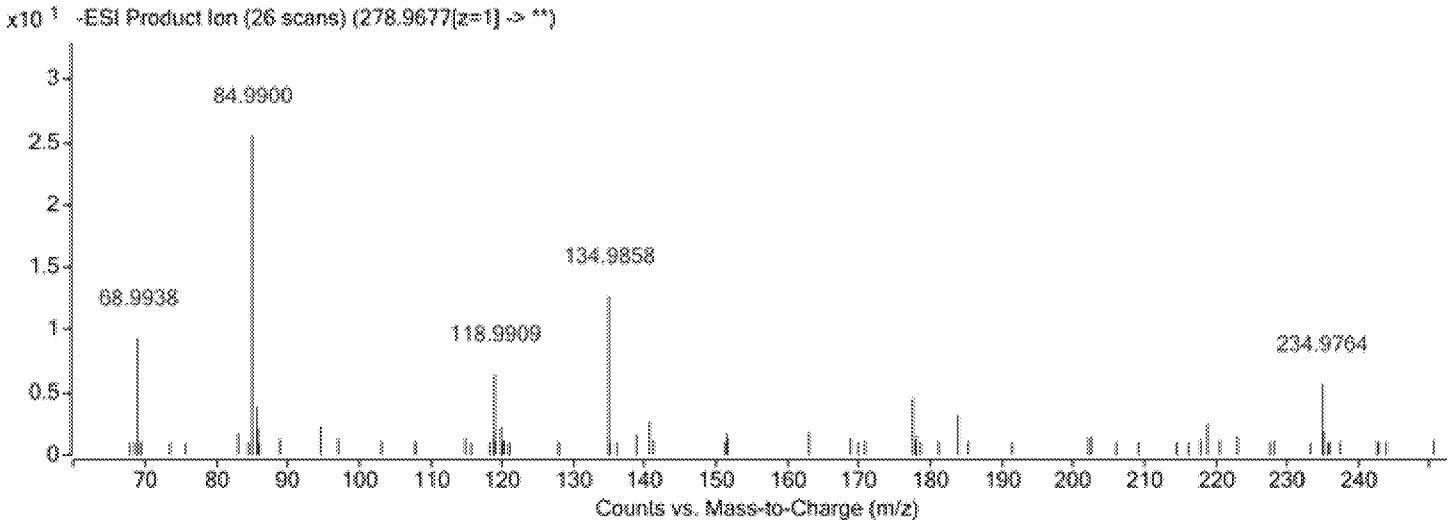
When I was doing structural determination on the Chemours Outfall back in May I was able to resolve the two for the PMPA/PFMOPrA you are discussing. See figure below from the manuscript in prep.



For PEPA/PFMOBA I was only able to detect one chromatographic peak (below)



but the MS/MS contains CF3/CF3O (68.99/84.99) and C2F5/C2F5O (118.99/134.99) (below) which is consistent with a mix of PEPA structure from Chemours and the Sun paper.



From: Detlef Knappe [mailto:knappe@ncsu.edu]
Sent: Friday, May 25, 2018 7:52 AM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Cc: Hopkins, Zachary <zrhopkin@ncsu.edu>; Nadine Kotlarz <nkotlar@ncsu.edu>; Chuhui Zhang <czhang24@ncsu.edu>; McCord, James <mccord.james@epa.gov>
Subject: Re: Package Delivery

Sure do!
So should the strategy be to sum linear and branched peaks if we get distinguishable signals?

On Fri, May 25, 2018, 7:48 AM Strynar, Mark <Strynar.Mark@epa.gov> wrote:

> Strynar, Mark has shared a OneDrive for Business file with you. To view it, click the link below.
>
> PEPA and PMPA structures.pptx

Detlef,

Do you recall when Mei's paper was published we had a discussion about PFMOPrA and PFMOBA being drawn incorrectly for the structures in Figure S1. We did not have standards so we had no way to tell. I believe they are one in the same. PFMOPrA is PMPA and PFMOBA is PEPA. In my 2015 paper I had the PMPA drawn right (Figure S5) but the PEPA wrong (Figure S5).

There MAY still be linear and branched isomers. We can do more QTOF work and run some HILIC methods to see if we get two peaks for these masses. However like PFOS and PFOA have isomers I don't think it is important.

See the attached PPT file

Mark

From: zrhopkin@ncsu.edu [mailto:zrhopkin@ncsu.edu]
Sent: Friday, May 25, 2018 6:54 AM
To: Detlef R. U. Knappe <knappe@ncsu.edu>
Cc: Nadine Kotlarz <nkotlar@ncsu.edu>; Chuhui Zhang <czhang24@ncsu.edu>; Strynar, Mark <Strynar.Mark@epa.gov>; McCord, James <mccord.james@epa.gov>
Subject: Re: Package Delivery

If I recall correctly the secondary ion was showing up. This suggested the branched form was present? I would need to compare the MS file parameters for the two in order to see what is different. If they are different then I could test the PFMOBA parameters on the PEPA.

Best,

Zack Hopkins

PhD student

Graduate Research Assistant

Mann Hall 319A Office

Civil, Construction, and Environmental Engineering

North Carolina State University

Raleigh, NC 27695

zrhopkin@ncsu.edu

301-518-7697

On May 24, 2018, at 11:56 PM, Detlef Knappe <knappe@ncsu.edu> wrote:

> But you were able to see PEPA before, correct? And could distinguish from PFMOBA, I think...
>
> On Thu, May 24, 2018 at 11:11 PM, Zachary Hopkins <zrhopkin@ncsu.edu> wrote:
>
> > Detlef,

My understanding is that these are the compounds PMPA and PEPA. We were provided both of these as 0.1% solutions in water.

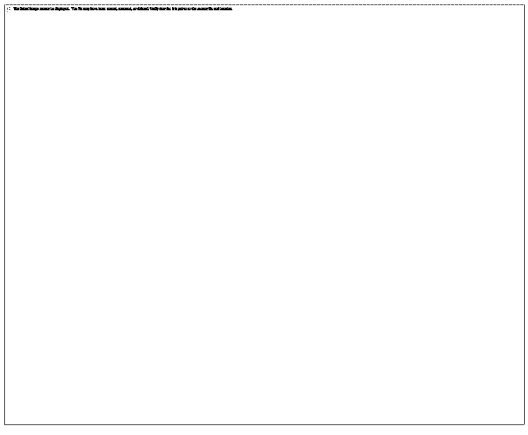
I have infused both of these on the triple quad. However, once I ran a calibration curve I could not detect them.

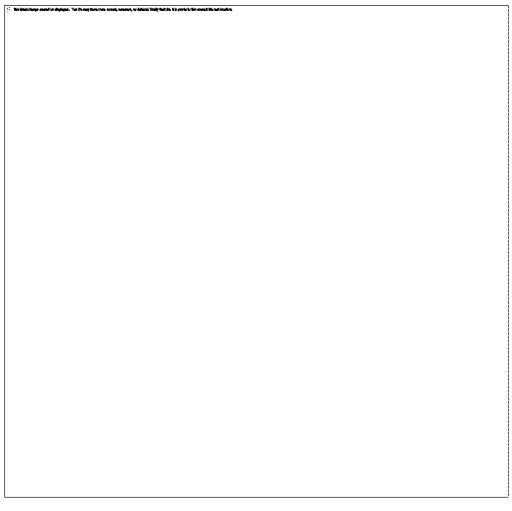
Best,

Zack

On Thu, May 24, 2018 at 7:25 PM, Detlef Knappe <knappe@ncsu.edu> wrote:

> Hi all,
>
> Do we have these compounds?





I know we have the linear methoxy versions, but I don't know whether Chemours sent the branched isomers.

Best,

Detlef

On Mon, May 7, 2018 at 5:18 PM, Nadine Kotlarz <nkotlar@ncsu.edu> wrote:

Zack,

The standards we recently received from Chemours were at 1000 ng/uL in water. I prepared 10 ng/uL aqueous stocks for each compound. Then I prepared a 1 ng/uL combined stock with:

1. PFO2HxA
2. NVHOS
3. PFO5DoA
4. PFO4DA
5. PFO3OA
6. PEPA
7. PMPA
8. Nafion byproduct 4

in water.

I already had a 1 ng/uL combined stock of GenX, PFMOAA, Nafion byproduct 1 and Nafion byproduct 2 in methanol. We prepared these standards with solids from Chemours a while ago. We decided we will make our calf serum calibration curves by dosing in the methanol and aqueous mixtures separately.

You're welcome to use any of the dilutions you want. They're stored in the cabinet to the bottom left of Mark's work space in the lab with the triple quad.

Nadine

On Wed, May 2, 2018 at 2:16 PM, Nadine Kotlarz <nkotlar@ncsu.edu> wrote:

> Sounds good. I'll bring the standards over to EPA tomorrow morning.
>
> On Wed, May 2, 2018 at 2:14 PM, Detlef Knappe <knappe@ncsu.edu> wrote:
>
> > Cool. And the PFO5DoA is included! Great for the blood work, Nadine :) My understanding is that Chemours didn't send this compound to Mark. Let's make sure it gets included in the method development.
> >
> > Detlef
> >
> > Detlef
> >
> > On Wed, May 2, 2018, 9:15 AM Zachary Hopkins <zrhopkin@ncsu.edu> wrote:
> >
> > > Detlef,
> > >
> > > Picked the standards up. We have the following now.
> > >
> > > PFHO2HxA
> > >
> > > PFMOAA
> > >
> > > PFO5DoA
> > >
> > > PFO4DA
> > >
> > > PFO3OA
> > >
> > > PEPA
> > >
> > > PMPA
> > >
> > > PFESA Byproduct 1
> > >
> > > PFESA Byproduct 2

PFESA Byproduct 4

NVHOS

Best,

Zack

On Wed, May 2, 2018 at 10:04 AM, Detlef Knappe <knappe@ncsu.edu> wrote:

> Zack,
>
> See below.
>
> The standards!
>
> Detlef
>
> ---------- Forwarded message ---------
> From: Barbara Simerson <bjsimers@ncsu.edu>
> Date: Wed, May 2, 2018, 6:55 AM
> Subject: Package Delivery
> To: Detlef Knappe <knappe@ncsu.edu>
>
> A package from Chemours was received addressed to you.

--

Barbara Simerson

Bookkeeper

North Carolina State University
Civil, Construction, and Environmental Engineering
2501 Stinson Drive/ 208 Mann Hall

Campus Box 7908
Raleigh, NC 27695
Phone: 919-515-7628
Fax: 919-515-7908

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Best,

Zack Hopkins

PhD student

Graduate Research Assistant

Mann Hall 319A Office

Civil, Construction, and Environmental Engineering

North Carolina State University

Raleigh, NC 27695

zrhopkin@ncsu.edu

301-518-7697

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Best,

Zack Hopkins

PhD student

Graduate Research Assistant

Mann Hall 319A Office

Civil, Construction, and Environmental Engineering

North Carolina State University

Raleigh, NC 27695

zrhopkin@ncsu.edu

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